

**PORTIONS  
OF THIS  
DOCUMENT  
ARE  
ILLEGIBLE**

**BLANK PAGE**

LA-UR-78-1521

MASTER


**TITLE:** INTERVALENCE BAND ABSORPTION IN ELECTRON  
HOLE DROPLETS

**AUTHOR(S):** R. N. Silver and C. H. Aldrich

**SUBMITTED TO:** 14th International Conference  
on the Physics of Semiconductors,  
Edinburgh, Scotland, September  
4 - 8, 1978.

By acceptance of this article the publisher re-  
squares that the U.S. Government retains a non-  
exclusive, royalty free license to publish or repro-  
duce the published form of this contribution, or to  
allow others to do so, for U.S. Government  
purposes.

The Los Alamos Scientific Laboratory requests that  
the publisher identify this article as work performed  
under the auspices of the Department of Energy.

  
**los alamos**  
**scientific laboratory**  
of the University of California  
LOS ALAMOS NEW MEXICO 87545

An Affirmative Action Equal Opportunity Employer

DEPARTMENT OF ENERGY  
CONTRACT W-740-ENG-16

**INTERVALENCE BAND ABSORPTION IN  
ELECTRON HOLE DROPLETS**

**by**

**R. N. Silver**  
**Theoretical Division, Los Alamos Scientific Laboratory**  
**University of California**  
**Los Alamos, New Mexico 87545**

**and**

**C. H. Aldrich**  
**M-Division, Los Alamos Scientific Laboratory**  
**University of California**  
**Los Alamos, New Mexico 87545**

**ABSTRACT**

**The broad absorption lineshape observed for transitions between the heavy hole and spin orbit split bands in EHD in Ge is explained. It is due to the momentum spreading of the hole wave function as calculated by multiple scattering theory.**

## INTERVALENCE BAND ABSORPTION IN ELECTRON HOLE DROPLETS

R N Silver, C H Aldrich  
MS 457 Los Alamos Scientific Laboratory  
Los Alamos, New Mexico 87545

The broad absorption lineshape observed for transitions between the heavy hole and spin orbit split bands in EHD in Ge is explained. It is due to the momentum spreading of the hole wave function as calculated by multiple scattering theory.

Pokrovsky et. al.<sup>1</sup> have observed a broad absorption due to transitions between the heavy hole and spin orbit split bands in Ge. It is much wider than predicted by the free particle theory which has successfully explained the lineshape for EHD luminescence. Similarly wide absorption is also observed for holes bound into excitons or to acceptors. In the latter case, Smith et. al.<sup>2</sup> have explained the lineshape in terms of the momentum spreading of the hole bound state wave function. In EHD or in degenerately doped semiconductors the screening is sufficiently large that bound states are absent. We present the first explanation of the lineshape in these systems.

In a simplified model where the potential acts only on holes in a spherical heavy hole band, the absorption is

$$\sigma(h\nu) \sim \sum_i f(\epsilon_i) \int d^3k |k|^2 |M|^2 |\langle k|\psi_i\rangle|^2 \delta(h\nu - \epsilon_k^{so} + \epsilon_i) \quad (1)$$

where the  $\psi_i$  are acceptor or exciton wave functions in the bound state case, and become plane wave states  $|k\rangle$  in the free hole theory. A comparison of the free hole theory including the effect of mass anisotropy with experiment is shown as the dashed line of Fig. 1. Intervalence band transitions conserve momentum (direct transition) and the occupied states in the heavy hole band are restricted to momenta less than the Fermi momentum. Thus, a sharp cutoff is predicted in the free hole theory for energies about 25 meV above the threshold for the transition. This conclusion is not altered by the inclusion of some many body effects such as final state interactions or renormalization

of the hole energy. We show that the momentum spreading of the hole wave function due to multiple scattering can explain the high energy tail observed experimentally.

Consider the simpler problem of the effect of impurity scattering on the absorption. The problem then is the choice of  $|\psi_i\rangle$  in (1). We propose a wave function based on the idea of a "coherent wave" in multiple scattering theory<sup>5</sup>. In the presence of uncorrelated scatterers a plane wave state is attenuated and the effective wave vector is shifted. This may be expressed by the addition to the energy  $\epsilon_k$  of a plane wave state of a self energy  $\Sigma(k)$  given by  $n_I \langle k|V|\psi_k^0\rangle$ . Here  $|\psi_k^0\rangle$  denotes a scattering wave function for a single impurity,  $|k\rangle$  a plane wave state, and  $n_I$  is the impurity density. This is the same as the well known relation of self energy to the forward scattering amplitude. Then we propose a multiple scattering wave function

$$\langle k|\psi_k^H\rangle = (2\pi)^3 \delta(\vec{k}-\vec{k}') - \frac{\sum_j e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_j} \langle \vec{k}|V|\psi_k^0\rangle}{\epsilon_k + \Sigma(\vec{k}) - \epsilon_k} \quad (2)$$

Note that in the limit of a single impurity (2) reduces to the usual expression for the projection of a scattering state onto a plane wave state with  $\Sigma(k)$  becoming  $\langle k|V|\psi_k^0\rangle$ . The sum over  $\vec{r}_j$  runs over all the impurities.

Now substitute (2) into (1) and average over the impurity positions. The terms which are singular as  $k \rightarrow k'$  exactly cancel, with the result

$$\sigma(\hbar\nu) = 2n_I \int \frac{d^3k}{(2\pi)^6} f(\epsilon_k) \int \frac{d^3k' |k|^2 |M|^2 |\langle \vec{k}|V|\psi_k^0\rangle|^2 \delta(\hbar\nu - \epsilon_k^{so} + \epsilon_{k'})}{(\epsilon_k - \epsilon_{k'} + \text{Re } \Sigma(k))^2 + (\text{Im } \Sigma(k))^2} \quad (3)$$

This expression contains the effect of the momentum spreading of the hole wave function which is responsible for the lineshape in the bound state case. It also contains the broadening of plane wave states due to multiple scattering. One may prove with the aid of the optical theorem that in

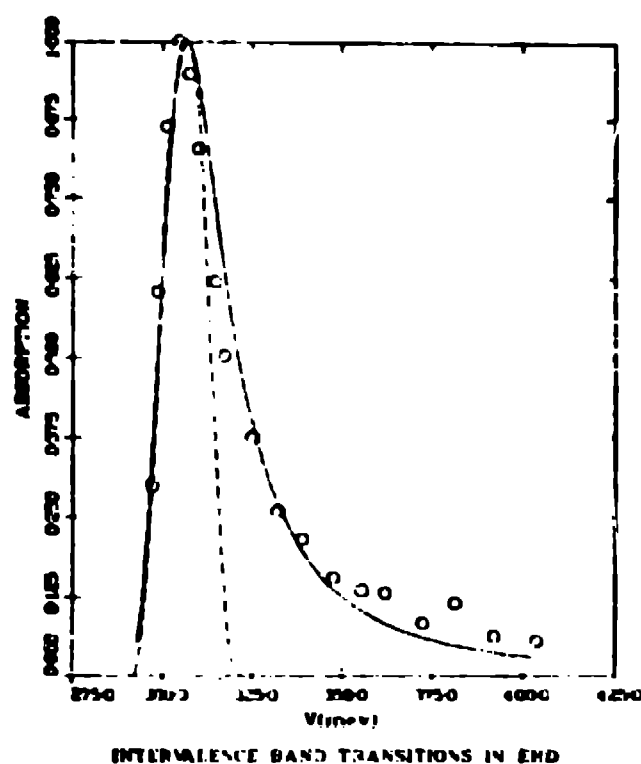


Fig 1. Data points are from Pokrovsky et. al. Dashed line is the free hole theory. Solid line is the present multiple scattering theory.

the limit of no scattering (3) goes to the free hole theory.

These ideas may be generalized to electron hole droplets by replacing impurity scattering by electron and hole scattering. We have carried out a calculation of this kind in the Born approximation with a static Yukawa screened interaction. The fit shown as the solid line in Fig 1 was obtained with a screening momentum of about one-half the Thomas Fermi value. Qualitative agreement with the slowly decreasing absorption tail at high energies is obtained. Other approximations made in this calculation are (i) the conduction and valence bands are taken to be spherical with density of states masses; (ii) absorption due to the light hole band is ignored; (iii) scattering effects in the spin orbit split band and the coupling between spin orbit and heavy hole bands due to the coulomb interaction are ignored; (iv) the matrix element  $M$  which is normally anisotropic is taken to be constant.

A calculation in which the Yukawa potential is replaced by

Hydynamically screened potential such as given by the RPA is in progress. A careful comparison with the RPA will require inclusion of structure anisotropy, band coupling, and especially the effects of scattering in the spin orbit split band. The latter is necessary to insure the proper cancellation of the plasmon contribution at zero momentum transfer. All these effects will act to broaden the absorption. Since the absorption is sensitive to the high momentum components of the wave function, it will be an important test for theories of electron correlation.

In conclusion, we have presented the first explanation of intervalence band absorption in FHD to go beyond the free hole theory. Other direct transitions such as the gain spectra of highly excited or heavily doped direct gap semiconductors also show strong deviations from the predictions of free particle theories for lineshapes<sup>4</sup>. We expect that the same multiple scattering ideas will find application to these problems.

#### REFERENCES

1. Pokrovsky Ya F, Svistunova K I 1971 Fiz. Tverd. Tela **13** 2788 (Soviet Physics - Solid State **13** 2331, 1971)
2. Smith D L, Chen M, McGill T C 1976 Physical Review **B14** 3504-3510
3. Lax M 1951 Reviews of Modern Physics **23** 287-310
4. Gobel G 1974 Applied Physics Letters **24** 412-414;  
Leheny R F, Shah J 1977 Physical Review Letters **38** 511-514